

Conditions for successful data assimilation

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Abstract

We show that numerical data assimilation is feasible in principle for an idealized model only if an effective dimension of the noise is bounded; this effective dimension is bounded when the noises in model and data satisfy a certain natural balance condition. If this balance condition is satisfied, data assimilation is feasible even if the number of variables in the problem is huge. We then analyze several data assimilation algorithms, including particle filters and variational data assimilation. We show that a particle filter can successfully solve most of the data assimilation problems which are feasible in principle, provided the particle filter is well designed. We also compare the conditions under which variational data assimilation can be successful with the conditions for successful particle filtering. We draw conclusions from our analysis and discuss its limitations.

1 Introduction

Many applications in science and engineering require that the predictions of uncertain models be updated by information from a stream of noisy data (see e.g. [6, 11]). The model and data jointly define a conditional probability density function (pdf) $p(x^{0:n}|z^{1:n})$, where the discrete variable $n = 0, 1, 2, \dots$ can be thought of as discrete time, x^n is a real m -dimensional vector to be estimated, called the “state”, $x^{0:n}$ is a shorthand for x^0, x^1, \dots, x^n , and where the data sets z^n are a k -dimensional vectors ($k \leq m$). All the information we have about the state at time n is contained in this conditional pdf and a variety of methods are available for its study, e.g. the Kalman filter [18], the extended and ensemble Kalman filter [13], particle filters [11], or variational methods [4, 33]. Given a model and data, each of these algorithms will produce a result. We are interested in the conditions under which this result is reasonable, i.e. consistent with the real-life situation one is modeling.

Generally, we restrict the analysis to linear state space models driven by Gaussian noise and supplemented by a synchronous stream of data perturbed by Gaussian noise, i.e. the noisy data are available at every time step of the model and only then. We further assume that all model parameters (including the covariance matrices of the noise) are known, i.e. we consider the case of state estimation (not parameter estimation or combined state and parameter estimation). We study this class of problems because it can be examined in some generality and (we believe) can explain qualitatively its important aspects, but we also point out its limitations.

In section 2, we examine what can be expected for our Gaussian model in principle, without regard to a specific algorithm. We define an effective dimension of a Gaussian data assimilation problem and show that, unless this effective dimension is moderate, the uncertainty in the model and the data is excessive so that making reliable conclusions about the underlying process is impossible. We argue that realistic problems have a moderate effective dimension. Investigating the role of the effective dimension in data assimilation algorithms is the subject of the remaining part of the paper. We briefly review particle filters in section 3. In section 4, we use the results of [30] to find the conditions under which the optimal particle filter (which in the linear synchronous case coincides with the implicit particle filter) performs well, and compare these conditions to what can be done in principle. We conclude that optimal particle filters can solve many data assimilation problems even if the number of variables to be estimated is large. Building on the results in [2, 5, 31], another particle filter is shown to fail under realistic conditions. Thus, the implementation of particle filters is very important, since a poor implementation can lead to a poor performance even if the effective dimension is small. In section 5 we consider particle smoothing and variational data assimilation and show that these methods can only be successful under conditions which are comparable to what we observed in particle filtering. We discuss limitations of our analysis in section 6 and present conclusions in section 7.

To avoid confusion, we wish to point out here that the effective dimension defined in this paper is different from the effective dimension introduced in [2, 5, 30, 31]. The effective dimension in [2, 5, 30, 31] is connected to particle filters, whereas the effective dimension defined in this paper is a characteristic of the model and data stream, i.e. independent of the algorithm for data assimilation. We show in particular that the effective dimension (as defined here) is well-bounded for realistic models and that numerical data assimilation can be successful in these cases, even if the number of variables to be estimated is large (i.e. a moderate effective dimension in our sense can

imply a small effective dimension in the sense of [2, 5, 30, 31].

2 The effective dimension of linear Gaussian data assimilation problems

We consider autonomous, linear Gaussian state space models of the form

$$x^{n+1} = Ax^n + w^n \quad (1)$$

where $n = 0, 1, 2, \dots$ is a discrete time, A_n is a given $m \times m$ matrix and w^n are independent and identically distributed (iid) Gaussian random variables with mean zero and given covariance matrix Q , which we write as $w^n \sim \mathcal{N}(0, Q)$. The initial conditions may be random and we assume that their pdf is also Gaussian, i.e. $x^0 \sim \mathcal{N}(\mu_0, \Sigma_0)$, with both μ_0 and Σ_0 given. We assume further that the data satisfy

$$z^{n+1} = Hx^{n+1} + v^{n+1}, \quad (2)$$

where H is a given $k \times m$ matrix ($k \leq m$) and the $v^{n+1} \sim \mathcal{N}(0, R)$ are iid, where R is a given $k \times k$ matrix. The w^n 's and v^n 's are independent of each other.

In principle, but not necessarily in practice, the covariance matrix P_n of the state x^n conditioned on the data $z^{1:n}$ can be computed recursively, starting with $P_0 = \Sigma_0$:

$$\begin{aligned} X_n &= AP_nA^T + Q, \\ K_n &= X_nH^T(HX_nH^T + R)^{-1}, \\ P_{n+1} &= (I_m - K_nH)X_n, \end{aligned}$$

where I_m is the identity matrix of order m and the $m \times k$ matrix K is often called the ‘‘Kalman gain’’. This is the Kalman formalism. Under suitable conditions on the ranks of the several matrices (specifically, if the pair (H, A) is d -detectable and (A, Q) is d -stabilizable, see [22], pp. 90–91), the covariance matrix reaches a ‘‘steady state’’ so that

$$P_{n+1} = P_n = P = (I - KH)X,$$

where X is the unique positive semi-definite solution of the discrete algebraic Riccati equation (DARE)

$$X = AXA^T - AXH^T(HXH^T + R)^{-1}HXA^T + Q.$$

Note that the steady state value of the covariance matrix is independent of the initial covariance matrix Σ_0 and that the rate of convergence to this limit is at least linear, in many cases quadratic (see [22], p. 313). This means that, after a relatively short time, the samples of the state given the data are normally distributed with mean μ_n and covariance matrix P (the mean μ_n of the variables is not needed here, but it can also be computed using Kalman's formulas).

The Frobenius norm $\|P\|_F = (\sum_{ij} p_{ij}^2)^{1/2}$ of the covariance matrix $P = (p_{ij})$ determines how far these samples spread out in the state space. To see this, consider the random variable $y = (x_n - \mu_n)^T(x_n - \mu_n)$, where $x_n - \mu_n \sim \mathcal{N}(0, P)$, i.e. consider the squared distances of the samples from their mean (their most likely value). Let U be an orthogonal $m \times m$ matrix whose columns are the eigenvectors of P . Then

$$y = (x_n - \mu_n)^T(x_n - \mu_n) = s^T s = \sum_{j=1}^m s_j^2,$$

where $s = U^T(x_n - \mu_n) \sim \mathcal{N}(0, \Lambda)$, and $\Lambda = U^T P U$ is a diagonal matrix whose diagonal elements are the m eigenvalues λ_j of P . It is now straightforward to compute the mean and variance of y because the s_j 's (the elements of s) are independent :

$$E(y) = \sum_{j=1}^m \lambda_j, \quad \text{var}(y) = 2 \sum_{j=1}^m \lambda_j^2.$$

Note that $y = r^2$, where r is the distance from the sample to the most likely state (the mean). Assuming that m is finite (but large), we obtain, using Taylor expansion of $r/\sqrt{\sum \lambda_j} = (z/\sqrt{\sum \lambda_j})^{1/2}$ around $\sqrt{\sum \lambda_j}$ and assuming that $\lambda_j = O(1)$, that

$$\begin{aligned} E(r) &= \frac{4 \left(\sum_{j=1}^m \lambda_j \right)^2 - 2 \sum_{j=1}^m \lambda_j^2}{4 \left(\sum_{j=1}^m \lambda_j \right)^{1.5}} + O_p \left(\frac{\sum_{j=1}^m \lambda_j^4}{\left(\sum_{j=1}^m \lambda_j \right)^4} \right) = \hat{E}(r) + O_p \left(\frac{\sum_{j=1}^m \lambda_j^4}{\left(\sum_{j=1}^m \lambda_j \right)^4} \right), \\ \text{var}(y) &= \frac{\sum_{j=1}^m \lambda_j^2}{2 \sum_{j=1}^m \lambda_j} + O_p \left(\frac{\sum_{j=1}^m \lambda_j^4}{\left(\sum_{j=1}^m \lambda_j \right)^3} \right) = \hat{v}(r) + O_p \left(\frac{\sum_{j=1}^m \lambda_j^4}{\left(\sum_{j=1}^m \lambda_j \right)^3} \right). \end{aligned}$$

Using the techniques in [5], one can show that for $m \rightarrow \infty$ and $\sum \lambda \rightarrow \infty$ and with $\lambda_j = O(1)$ (i.e. in the case for which the moments of y do not necessarily exist) the above expressions become “ $Asmean(r)$ ” respectively “ $Asvar(r)$ ”, i.e. the moments of limiting Gaussian variables.

Now suppose that m is large but finite and that $\lambda_j = O(1)$ for $j = 1, \dots, m$; then $\hat{E} = O(m^{1/2})$ and $\hat{v} = O(1)$. This means that the samples collect on a shell of thickness $O(1)$ at a distance $O(m^{1/2})$ from their mean and are distributed over a volume $O(m^{(m+1)/2})$, i.e. the predictions spread out over a large volume at a large distance from the most likely state. However, the data assimilation problem reflects an experimental situation, and the numerical samples should behave just like experimental samples: if the uncertainty is large, one will observe that the outcomes of repeated experiments exhibit a large spread; if the uncertainty is small, then the spread in the outcomes of experiments is also small. Since the outcomes of repeated experiments rarely exhibit large variations, one should expect that the samples of numerical data assimilation all fall into a small “low-dimensional” ball, centered around the most likely state, i.e. the radius, $E(r) \approx \hat{E}$, is comparable to the thickness, $var(r) \approx \hat{v}$. Data assimilation only makes sense in this case because, otherwise, the samples spread out over a huge volume and there is not enough information in the model and data to make reliable conclusions about the state.

Standard inequalities show that

$$\sqrt{\sum_{j=1}^m \lambda_j^2} \leq \sum_{j=1}^m \lambda_j \leq \sqrt{m \sum_{j=1}^m \lambda_j^2},$$

and now one can obtain upper bounds for \hat{E} and \hat{v} :

$$\hat{E} \leq m \left(\sum_{j=1}^m \lambda_j^2 \right)^{1/4}, \quad \hat{v} \leq \frac{1}{2} \left(\sum_{j=1}^m \lambda_j^2 \right)^{1/2}.$$

These upper bounds imply that the sum of the eigenvalues squared of the steady state covariance matrix P , i.e. its Frobenius norm, determines the mean and variance of the distance of a sample from the most likely state, i.e. the spread of the samples in the state space. We thus define the *effective dimension* of the Gaussian data assimilation problem defined by equations (1) and (2) to be the Frobenius norm of P , $\|P\|_F = \sqrt{\sum \lambda_j^2}$.

Note that this effective dimension is different from the definitions in [2, 5, 30, 31], which are defined in connection with specific particle filters.

The effective dimension defined here is independent of a data assimilation technique; it is a characteristic of the model (1) and data stream (2). We expect the effective dimension to be bounded in practice and corroborate this point in the next two sections.

Finally we want to point out that we study the posterior pdf (the pdf of x conditioned on the data); this pdf can be calculated with the Kalman filter formulas, which however are valid only for linear Gaussian models as in (1) and (2). Nonlinear or non-Gaussian models are not discussed here, but we mention the limitations of our analysis in more detail in section 6.

2.1 Bounds on the effective dimension

To discover the real-life interpretation of the effective dimension, we study its upper bounds in terms of the Frobenius norms of Q and R . From Khinchin's theorem [8] we know that the Frobenius norms of Q and R must be bounded or else the energy of the noise is infinite (which is unrealistic). Here, we show that a small Frobenius norm of Q and R can lead to a small effective dimension. We start by a simple example, which is also useful in the study of data assimilation methods in later sections.

2.1.1 Example

Put $A = H = I_m$ and let $Q = qI_m$, $R = rI_m$. The Riccati equation can be solved analytically for this example and we find that the Frobenius norm of the steady state covariance is

$$\|P\|_F = \sqrt{m} \frac{\sqrt{q^2 + 4qr} - q}{2}.$$

In a real-life problem, we would expect $\|P\|_F$ to grow slowly, if at all, when the number of variables increases. The boundedness of the effective dimension induces a “balance condition” between the errors in the model (represented by q) and the errors in the data (represented by r). In this simple example, this balance condition is the inequality

$$\frac{\sqrt{q^2 + 4qr} - q}{2} \leq \frac{1}{\sqrt{m}},$$

where the 1 in the numerator of the right-hand side stands for a constant $O(1)$, or even for a function of m that grows slower than \sqrt{m} ; we set this constant equal to 1 because this already captures the general behavior. Figure 1 illustrates the balance condition and shows a plot of the function that

is defined by the left-hand-side of the above inequality as well as three level sets, corresponding to $m = 5, 10, 100$ respectively; for a given dimension m , all values of q and r below the corresponding level set lead to an $O(1)$ effective dimension.

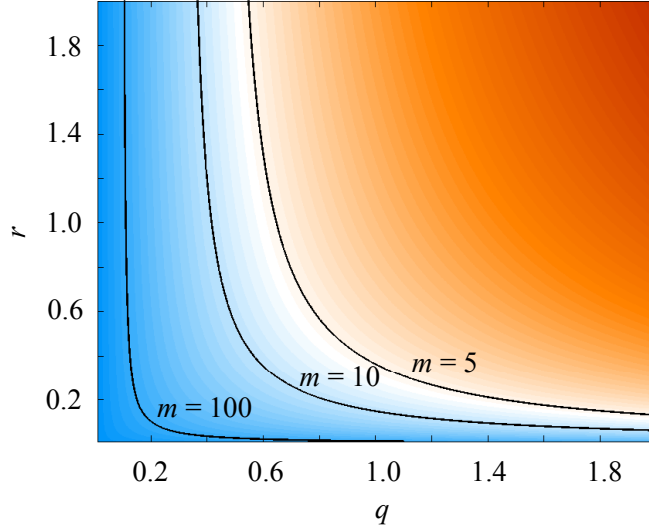


Figure 1: Covariance map for sequential data assimilation.

The balance condition in this model problem implies that the smaller the errors in the data (r), the larger can be the uncertainty in the model (q) and vice versa, and, for large m , only small values of q and r are allowed. Moreover, note that for very small q , the boundaries for successful data assimilation are (almost) vertical lines. The reason is that if the model is very good, neither accurate nor inaccurate data can improve it, i.e. data assimilation is not necessary. If the model is poor, only nearly perfect data can help. We will encounter this balance condition (in more complicated forms) again in the general case in the next section and also in the analysis of particle filters and variational data assimilation.

Finally, note that the Frobenius norms $\|Q\|_F = q\sqrt{m}$ and $\|R\|_F = r\sqrt{m}$ increase with the number of dimensions unless q or r or both decrease with m as shown in figure 1. We will argue in section 2.2 that in realistic cases, the Frobenius norms of Q and R remain bounded as m increases. We also expect, but cannot prove in general, that a balance condition as in figure 1 is valid in the general case (arbitrary A, H, Q, R), with q and r replaced by

the Frobenius norms of Q and R .

2.1.2 The general case

In the general case, the balance condition between the uncertainties in the model ($\|Q\|_F$) and data ($\|R\|_F$) is more complicated because the effective dimension is the Frobenius norm of the solution of a Riccati equation which in general does not admit a closed form solution.

However, if the covariance matrices Q and R have small Frobenius norms, then the effective dimension of the problem can be small and data assimilation can be successful. To see this, let X and P be the solution of the DARE respectively the steady state covariance matrix of a given (A, Q, H, R) data assimilation problem and let $\tilde{Q} \leq Q$, i.e. $\tilde{Q} - Q$ is symmetric positive semi-definite (SPD). If $\tilde{R} \leq R$, then, by the comparison theorem (Theorem 13.3.1) in [22], $\tilde{X} \leq X$, where \tilde{X} is the solution of the DARE associated with the $(A, \tilde{Q}, H, \tilde{R})$ data assimilation problem. From the Kalman formulas we know that

$$P = X - XH^T(HXH^T + R)^{-1}HX,$$

which implies that $P \leq X$. Moreover, for two SPD matrices C and D , $C \leq D$ implies $\|C\|_F \leq \|D\|_F$. Thus, the smaller the Frobenius norm of Q and R , the smaller is the upper bound $\|X\|_F$ on the effective dimension.

However, the requirement that these Frobenius norms be small is not sufficient to ensure that the effective dimension of the problem is small; in particular, it is evident that the properties of A must play a role; for example, if the L_2 norm of A exceeds unity, the model (1) is unstable and successful data assimilation is unlikely.

While the model, or A , is implicitly accounted for in X , the solution of the DARE, one can construct sharper bounds on the effective dimension by accounting for the model (1) and data stream (2) more explicitly. To that extend, we construct matrix bounds on P , from matrix bounds for the solution of the DARE [21]. Let $X \leq X_u$, and $X_l \leq X$, be upper and lower matrix bounds for the solution of the DARE, for example, we can choose the lower bound in [20]

$$Q \leq X_l = A(Q^{-1} + H^T R^{-1} H)^{-1} A^T + Q \leq X,$$

and the upper bound in [21]

$$X \leq X_u = A(X_*^{-1} + H^T R^{-1} H)^{-1} A^T + Q,$$

where $X_* = A(\eta^{-1} + H^T R^{-1} H)^{-1} A^T + Q$, $\eta = f(-\lambda_1(A) - \lambda_n(H^T R^{-1} H) \lambda_1(Q) + 1, 2\lambda_n(H^T R^{-1} H), 2\lambda_1(Q))$, $f(a, b, c) = (\sqrt{a^2 + bc} - a)/2$ and $\lambda_1(C)$ and $\lambda_n(C)$ are the largest respectively smallest eigenvalue of the matrix C . Then an upper matrix bound for the steady state covariance matrix is

$$P \leq X_u - X_l H^T (H X_u H^T + R)^{-1} H X_l.$$

The Frobenius norm of this upper matrix bound is an upper bound for the effective dimension.

2.2 The real-world interpretation of effective dimension

We have shown that there is little hope for making reliable conclusions unless the effective dimension of the data assimilation problem defined by equations (1) and (2) is small. We now give more detail about the physical interpretation of this result.

Suppose the variables x one is estimating are point values of, for example, the velocity of a flow field (as they often are in applications). The Frobenius norm of the covariance matrix Q is proportional to the specific kinetic energy of the noise field that is perturbing an underlying flow. This energy should be a small fraction of the energy of the flow, or else there is not enough information in the model (1) to examine the flow one is interested in. We can thus assume that the Frobenius norm of Q is (much) less than m . By the same arguments, we can assume that the Frobenius norm of R is small, or else the noise in the data equation overpowers the actual measurements. Since small Frobenius norms of Q and R often imply a small Frobenius norm of P , we are dealing with a data assimilation problem with a small effective dimension.

Point values of a flow field typically come from a discretization of a stochastic differential equation. As one refines this discretization, one can expect the correlation between the errors at neighboring grid-points to increase. These errors are represented by the covariance matrix Q and from Khinchin's theorem (see e.g. [8]) we know that a random field with sufficiently correlated components has a finite energy density (and vice versa). This implies that the Frobenius norm of Q does not grow without bound as we increase m .

Another and perhaps even more dramatic instance of this situation is one where the random process we are interested in is smooth so that the spectrum of its covariance matrix decays quickly [1, 28]. For practical purposes one may then consider $m - d$ of the eigenvalues to be equal to zero

(rather than just very small). This is an instance of “partial noise” [26], i.e. the state space splits into two disjoint subspaces, one of dimension d , which contains state variables, u , that are directly driven by Gaussian noise, and one of dimension $m - d$, which contains the remaining variables, v , that are (linear) functions of the random variables u . Thus, the steady state covariance matrix is of size $d \times d$ and the effective dimension is independent of the state dimension and moderate even if m is large.

Note that the key to the small effective dimension in the above cases is the correlation among the errors and indeed, the data assimilation problems (or covariances Q and R) derived by various practitioners and theorists show a strong correlation of the errors (see e.g. [1, 3, 14, 24–26, 28, 29, 34, 40]). The correlations are also key to the well-boundedness of infinite dimensional problems [32] where the spectra of the covariances (which are compact operators in this case) decay; a well correlated noise model was obtained from an infinite dimensional problem in [3, 7].

The geometrical interpretation of this situation is as follows: because of correlations in the noise, the probability mass is concentrated on a d -dimensional manifold, regardless of the dimension $m \geq d$ of the state space. In addition one must be careful that the noise in the observations not be too strong. Otherwise the data can push the probability mass away from the d -dimensional manifold (i.e. the data increase uncertainty, instead of decreasing it). This assumption is reasonable, because typically the data contain information and not just noise.

Next, suppose that the vector x in (1) and (2) represents the components of an abstract model with the several components representing various indicators, for example of economic activity (so that the concept of energy is not well-defined). It is unreasonable to assume that each source of error affects only one component of x . As an example of what happens when each source of error affects many components, consider a model where Gaussian sources of error are distributed with spherical symmetry in the space of the x ’s and have a magnitude independent of the dimension m . In an m dimensional space, the components of the unit vector of length 1 have magnitude of order $1/\sqrt{m}$, so that the variance of each component must decrease like $1/m$. Thus, the covariance matrices in (1) and (2) are proportional to $m^{-1}I_m$ and the effective dimension (for $A = H = I_m$) is $\|P\|_F = (\sqrt{5} - 1)/2m$, which is small when m is large. This is a plausible outcome, because the more data and indicators are considered, the less uncertainty there should be in the outcome (because the new indicators provide additional information).

3 Review of particle filters

In importance sampling one generates samples from a hard-to-sample pdf p (the “target” pdf) by producing weighted samples from an easy-to-sample pdf, π , called the “importance function” (see e.g. [8, 19]). Specifically, if the random variable one is interested in is $x \sim p$, one generates samples $X_j \sim \pi, j = 1, \dots, m$, (we use capital letters for realizations of random variables) and weighs each by the weight

$$W_j \propto \frac{p(X_j)}{\pi(X_j)}.$$

The weighted samples $\{X_j, W_j\}$ (called particles in this context) form an empirical estimate of the target pdf p , i.e. for a smooth function u , the sum

$$E_m(u) = \sum_{j=0}^m u(X_j) \hat{W}_j,$$

where $\hat{W}_j = W_j / \sum_{j=0}^M W_j$, converges almost surely to the expected value of u with respect to the pdf p as $m \rightarrow \infty$, provided that the support of π includes the support of p .

Particle filters apply these ideas to the recursive formulation of the conditional pdf:

$$p(x^{0:n+1} | z^{1:n+1}) = p(x^{0:n} | z^{1:n}) \frac{p(x^{n+1} | x^n) p(z^{n+1} | x^{n+1})}{p(z^{n+1} | z^{1:n})}.$$

This requires that the importance function factorize in the form:

$$\pi(x^{0:n+1} | z^{0:n+1}) = \pi_0(x^0) \prod_{k=1}^{n+1} \pi_k(x^k | x^{0:k-1}, z^{1:k}). \quad (3)$$

where the π_k are updates for the importance function. The factorization of the importance function leads to the recursion

$$W_j^{n+1} \propto \hat{W}_j^n \frac{p(X_j^{n+1} | X_j^n) p(Z^{n+1} | X_j^{n+1})}{\pi_{n+1}(X_j^{n+1} | X_j^{0:n}, Z^{0:k})}, \quad (4)$$

for the weights of each of the particles, which are then scaled so that their sum equals one. Resampling after every step makes it possible to set $\hat{W}_j^n = 1/m$ when one computes W_j^{n+1} (see e.g. [11]). Once one has set $\hat{W}_j^n = 1/m$

but before sampling, each of the weights can be viewed as a function of the random variable x_j^{n+1} and is therefore a random variable.

The weights determine the efficiency of particle filters. Suppose that, before the normalization and resampling step, one weight is much larger than all others; then upon rescaling of the weights such that their sum equals one, one finds that the largest normalized weight is near 1 and all others are near 0. In this case the empirical estimate of the conditional pdf by the particles is very poor (it is a single, often unlikely point) and the particle filter is said to have collapsed. The collapse of particle filters can be studied via the variance of the logarithm of the weights, and it was argued rigorously in [2,5,30,31] that a large variance of the logarithm of the weights leads to the collapse of particle filters. The choice of importance function π is critical for avoiding the collapse and many different importance functions have been considered in the literature (see e.g. [9, 10, 27, 35–38]). Here we follow [2, 5, 30, 31] and discuss two particle filters in detail.

3.1 The SIR filter

A natural choice for the importance function is to generate samples with the model (1), i.e. to choose $\pi_{n+1} = p(x^{n+1}|x^n)$. When a resampling step is added, the resulting filter is often called a sequential importance sampling with resampling (SIR) filter [15] and its weights are

$$W_j^{n+1} \propto p(Z^{n+1}|X_j^{n+1}).$$

It is known that the SIR filter collapses if the importance function $\pi_{n+1} = p(x^{n+1}|x^n)$, called the “prior”, and the target, or “posterior” density, $p(y^{n+1}|x^{n+1})p(x^{n+1}|x^n)$, are nearly mutually singular. This can happen even in one dimensional problems, however the situation becomes more dramatic as the dimension m increases. A rigorous analysis of the asymptotic behavior of weights of the SIR filter (as the number of particles and the dimension go to infinity) is given in [2, 5, 31] and it is shown that the number of particles required to avoid the collapse of the SIR filter grows exponentially with the variance of the observation log likelihood (the logarithm of the weights).

3.2 The optimal particle filter

One can avoid the collapse of particle filters in low-dimensional problems by choosing the importance function wisely. If one chooses an importance function π so that the weights in (4) are close to uniform, then all particles contribute equally to the empirical estimate they define. In [12, 23, 30, 39] the

importance function $\pi_{n+1}(x^{n+1}|x^{0:n}, z^{0:n+1}) = p(x^{n+1}|x^n, z^{n+1})$, is discussed and it is shown that this importance function is “optimal” in the sense that it minimizes the variance of the weights given the data *and* X_j^n . For that reason, a filter that uses this importance function is called “optimal particle filter” and the optimal weights are

$$W_j^{n+1} \propto p(Z^{n+1}|X_j^n). \quad (5)$$

For the class of models and data we consider, the optimal particle filter is identical to the implicit particle filter [9, 27]. The asymptotic behavior of the weights of the optimal particle filter was studied in [30] and it was found that the optimal filter collapses if the variance of the logarithm of its weights is large.

4 The collapse and non-collapse of particle filters

The conditions for the collapse have been reported in [2, 5, 31] for SIR and in [30] for the optimal particle filter; here we connect these to our analysis of effective dimension.

4.1 The case of the optimal particle filter

It was shown in [30], that the optimal particle filter collapses if the Frobenius norm of the covariance matrix of $(HQH^T + R)^{-0.5} H A x^{n-1}$ is large (asymptotically infinite as $k \rightarrow \infty$). However if this Frobenius norm is small, then the variance of the logarithm of the weights is also small so that the optimal particle filter works just fine (i.e. it does not collapse). We now investigate the role the effective dimension of section 2 plays for the collapse of the optimal particle filter.

If the conditional pdf has reached steady state, then the covariance of x^{n-1} is P (the steady state solution of the Riccati equation), so that the Frobenius norm of the symmetric matrix

$$\Sigma = H A P A^T H^T (H Q H^T + R)^{-1}, \quad (6)$$

governs the collapse of the optimal particle filter. If the Frobenius norm of Σ is well-bounded for large m and k , then the optimal particle filter will work. The boundedness of Σ induces a balance condition between the errors in the model and in the data; the situation is analogous to what we observed in section 2.

To understand this balance condition better, we consider again the simple example of section 2, i.e. we set $H = A = I_m$ and $Q = qI_m$, $R = rI_m$. We already computed P in section 2 and find from (6) that

$$\|\Sigma\|_F = \sqrt{m} \frac{\sqrt{q^2 + 4qr} - q}{2(q + r)}.$$

The boundedness of $\|\Sigma\|_F = O(1)$ thus induces the condition

$$\frac{\sqrt{q^2 + 4qr} - q}{2(q + r)} \leq \frac{1}{\sqrt{m}}.$$

With m fixed, the left-hand-side depends only on the ratio of the covariances of the noise in the model and in the data, so that the level sets are rays. In the center panel of figure 2, we superpose these rays, for which optimal particle filtering can be successful, with the (q,r)-region in which data assimilation is feasible (as computed in section 2). The left panel of the figure shows what is in principle possible, for comparison.

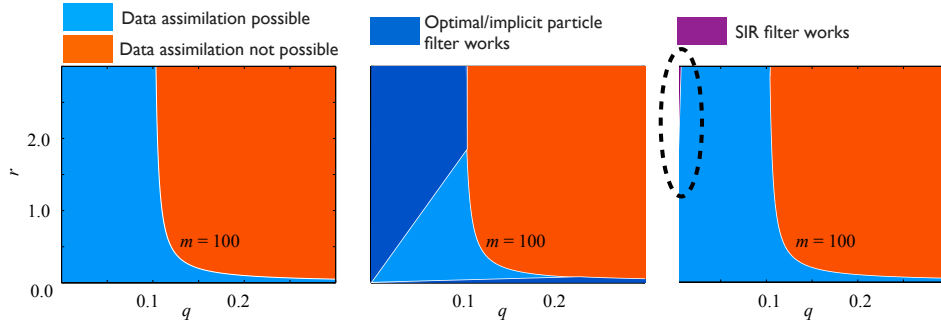


Figure 2: Covariance map for successful data assimilation (left panel), and two particle filtering algorithms (center and right panel). The broken ellipse in the right panel locates the area where the SIR filter works.

We find that the optimal particle filter can successfully solve many of the data assimilation problems that are well defined (in the sense that one can expect reliable conclusions given model and data, see section 2). The exception are problems for which $q \approx r$, i.e. the noise in the model and data are equally strong.

Another way to see this is to set $\epsilon = q/r$ so that the balance condition becomes

$$\frac{\sqrt{\epsilon^2 + 4\epsilon} - \epsilon}{2(1 + \epsilon)} \leq \frac{1}{\sqrt{m}},$$

which we solve for m and then plot the maximum dimension m as a function of the ratio of the noise in the model and the noise in the data; all values smaller than this maximum dimension are shown in figure 3 as the light blue area. We conclude that the optimal particle filter works for high-dimensional data

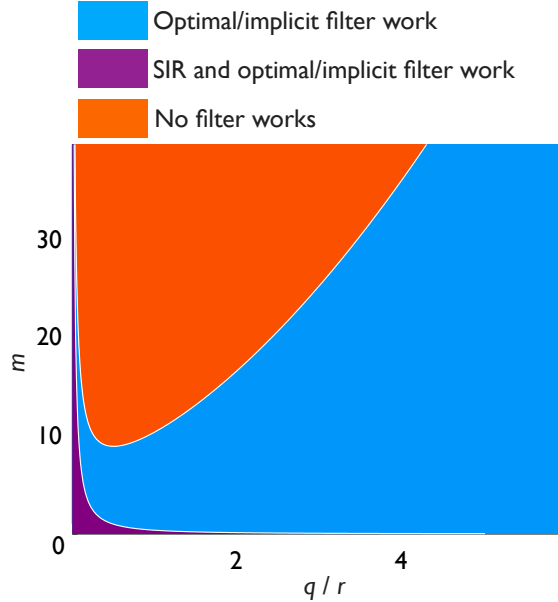


Figure 3: Maximum dimension for two particle filters.

assimilation problems if ϵ is either small or large. The case of large ϵ is the case typically encountered in practice. The reasons are as follows: if ϵ is small, then the model is very accurate. In this case, neither accurate nor inaccurate data can improve the model predictions (this case corresponds to the vertical line in figure 2), i.e. data assimilation is unnecessary since one can simply trust the predictions of the model (1). If ϵ is large, then the uncertainty in the data is much less than the uncertainty in the model, i.e. we can learn a lot from the data. This is the interesting case and the optimal particle filter (or the implicit particle filter) can be expected to work in such scenarios. However, problems occur when $\epsilon \approx 1$ and if the state dimension exceeds $m \approx 20$. We expect this case to occur infrequently, because typically the data are more accurate than the model.

It is however important to realize that the collapse of the optimal particle filter for $\epsilon \approx 1$ does *not* imply that Monte Carlo sampling in general

is not applicable in this case. Particle filtering induces variance into the weights because of its recursive problem formulation and this variance can be reduced by particle smoothing. The reason is as follows: the variance of the weights of the optimal particle filter depends only on the variance of the particles' positions at time n (see (5)), i.e. each particle is updated to time $n + 1$ such that no additional variance is introduced (this is why this filter is called optimal); however the positions at time n may be unlikely in view of the data at $n + 1$ (due to accumulation of errors up until this point). In this case, one can go back and correct the past, i.e. use a particle smoother (see also section 5). However, the number of steps one needs to go back in time for successful smoothing is problem dependent and, thus, we cannot provide a full analysis here (given that we work in a restrictive linear setting it seems more realistic and efficient to do this analysis on a case by case basis). In particular, it was indicated in two independent papers [37, 38] that smoothing a few steps backwards can help with making Monte Carlo sampling applicable in situations where particle filters fail. In [38], the low-noise regime (which is an instance of the case where $\epsilon \approx 1$) is considered in connection with an application in oceanography and it was found that particle smoothing is helpful, however the approximations for optimal particle smoothers become difficult and computationally expensive as the problems get nonlinear. In [37], particle smoothing was found to give superior results than particle filtering for combined parameter and state estimation, again in connection with an application in oceanography.

In the general case (arbitrary A, H, Q, R), we can simplify the balance condition for successful particle filtering by using the upper bound for the Frobenius norm of Σ :

$$\|\Sigma\|_F \leq \|A\|_F^2 \|H\|_F^2 \|P\|_F \| (HQH^T + R)^{-1} \|_F.$$

If we require that this upper bound is less than \sqrt{m} , then we find, using the upper bound

$$\sqrt{m} = \|I\|_F \leq \| (HQH^T + R) \|_F \| (HQH^T + R)^{-1} \|_F,$$

that

$$\|A\|_F^2 \|H\|_F^2 \|P\|_F \leq \|H\|_F^2 \|Q\|_F + \|R\|_F,$$

is a sufficient condition that the Frobenius norm of Σ is small (i.e. it grows slower than $O(\sqrt{m})$). As in section 2, we find that the balance condition in terms of $\|R\|_F$ and $\|Q\|_F$, is simple in simple cases, but delicate in general.

4.2 The case of the SIR filter

The collapse of the SIR filter has been studied in [2, 5, 31], and it was shown that, for a properly normalized model and data equation, this collapse is governed by the Frobenius norm of the covariance of Hx^n ; undoing the scaling, and noting that x^{n-1} has covariance P (the steady state solution of the Riccati equation), we find that the Frobenius norm of

$$\Sigma = H (Q + APA^T) H^T R^{-1}.$$

governs the collapse of SIR filters. Thus, the boundedness of $\|\Sigma\|_F$ is the balance condition for successful data assimilation with an SIR particle filter. For the simple example considered earlier ($A = H = I_m$, $Q = qI_m$, $R = rI_m$), this condition becomes

$$\frac{\sqrt{q^2 + 4qr} + q}{2r} \leq \frac{1}{\sqrt{m}}.$$

For $m = 100$, the (q,r)-region for which data assimilation with an SIR filter can be successful is plotted in the right panel of figure 2. We observe that this region is very small compared to the region that is accessible with an optimal particle filter.

We can also set $\epsilon = q/r$ and obtain

$$\frac{\sqrt{\epsilon^2 + 4\epsilon} + \epsilon}{2} \leq \frac{1}{\sqrt{m}},$$

which we solve for m so that we can plot the maximum dimension for which SIR particle filtering can be successful as a function of the covariance ratio ϵ (see figure 3). Again, we observe that the SIR particle can only be useful in a limited class of problems. In particular, we find that the SIR particle filter works in high-dimensional problems only if the model is very accurate (compared to the data). However, we argued before that this case is somewhat unrealistic, since we expect that the errors in the model be typically larger than the errors in the data (or else the data are not very useful, or particle filtering unnecessary because the model is very good). In these realistic scenarios, the SIR particle filter collapses and we conclude that, as the dimension m increases, it becomes more and more important to use the optimal importance function or a good approximation of it (see e.g. [27, 36–38] for approximations of the optimal filter).

In the general case, we can use an upper bound, e.g.

$$\|\Sigma\|_F \leq \|H\|_F^2 \|R^{-1}\|_F (\|Q\|_F + \|A\|_F^2 \|P\|),$$

and if we require that this bound is less than \sqrt{m} , we obtain the simplified balance condition

$$\|H\|_F^2 (\|Q\|_F + \|A\|_F^2 \|P\|) \leq \|R\|_F.$$

The above condition implies that the Frobenius norm of the covariance matrix of the model noise, Q , must be much smaller than the Frobenius norm of the covariance matrix of the errors in the data, which is unrealistic.

4.3 Discussion

We wish to point out differences and similarities of our work and the asymptotic studies in [2, 5, 30, 31]. Clearly, the results of [2, 5, 30, 31] are used in our analysis of the optimal particle filter (section 4.1) and the SIR filter (this section). Moreover, our analysis confirms Snyder’s findings in [30], where it was shown that the optimal particle filter “dramatically reduces the required sample size” (by lowering the exponent in the relation between the number of particles and the state dimension). In [2, 5, 30, 31], it was shown that the number of particles required grows exponentially with the variance of the logarithm of the weights; the variance of the logarithm of the weights if governed by the Frobenius norms of covariance matrices (which are different for SIR and the optimal particle filter). Our main contribution (in connection with particle filters) is to study the connection of these Frobenius norms with the effective dimension of section 2: if the effective dimension is well-bounded then these Frobenius norms do not necessarily grow with the state dimension m . Thus, we can find conditions under which the SIR and optimal particle filters can work. We also explain the physical interpretation of our results and conclude that the optimal particle filter can work for many realistic (and large dimensional) problems, because realistic conditions imply a moderate effective dimension.

5 Particle smoothing and variational data assimilation

We now consider the role of the effective dimension in particle smoothing and variational data assimilation. The idea here is to replace the step-by-step construction of the conditional pdf in a particle filter (or Kalman filter) by direct sampling of the full pdf $p(x^{0:n}|z^{1:n})$, i.e. all available data are assimilated in one sweep. Particle smoothers apply importance sampling to

obtain weighted samples from this pdf, and in variational data assimilation one estimates the state of the system by the mode of this pdf.

It is clear that either method can only be successful if the Frobenius norm of the covariance matrix of the variables conditioned on the data is small, or else the samples of numerical or physical experiments collect on a thin shell far from the most likely state (to obtain this result, one has to repeat the steps in section 2). We now determine the conditions under which this Frobenius norm is small. As is customary in data assimilation, we distinguish between the “strong constraint” and “weak constraint” problem.

5.1 The strong constraint problem

In the strong constraint problem one considers a “perfect model”, i.e. the model errors are neglected and we set $Q = 0$ (see e.g. [33]). Since the initial conditions determine the state trajectory, the goal is to obtain initial conditions that are compatible with the data, i.e. we are interested in the pdf

$$p(x^0|z^{1:n}) \propto \exp\left(-\frac{1}{2}(x^0 - \mu_0)^T \Sigma_0^{-1}(x^0 - \mu_0)\right) \\ \times \exp\left(-\frac{1}{2}\sum_{j=1}^n (z^j - HA^j x^0)^T R^{-1}(z^j - HA^j x^0)\right).$$

Straightforward calculation shows that this pdf is Gaussian (under our assumptions) and its covariance matrix is

$$\Sigma^{-1} = \Sigma_0^{-1} + \sum_{j=1}^n (A^j)^T H^T R^{-1} H A^j.$$

As explained above, data assimilation for the Gaussian model makes sense only if the Frobenius norm of this matrix is small (or at least, if it does not grow with the state dimension). In this case, the samples collect on a small and low-dimensional ball, close to the most likely state. The boundedness of the Frobenius norm of Σ induces a balance condition between the prior errors (Σ_0) and the errors on the data (R). The situation is analogous to the balance conditions we encountered before in sequential data assimilation.

We illustrate the balance condition for the strong constraint problem by considering a version of the simple example we used earlier, i.e. we set $A = H = I_m$, $Q = 0$, $R = rI_m$, and, in addition, $n = 1$, $\Sigma_0 = \sigma_0 I_m$. In this

case, we can compute Σ and its Frobenius norm:

$$\|\Sigma\|_F = \sqrt{m} \frac{\sigma_0 r}{\sigma_0 + r}.$$

Figure 4 shows the values of r and σ_0 which lead to an $O(1)$ Frobenius norm of Σ . Three level sets indicate the state dimensions $m = 10, 100, 1000$; for a

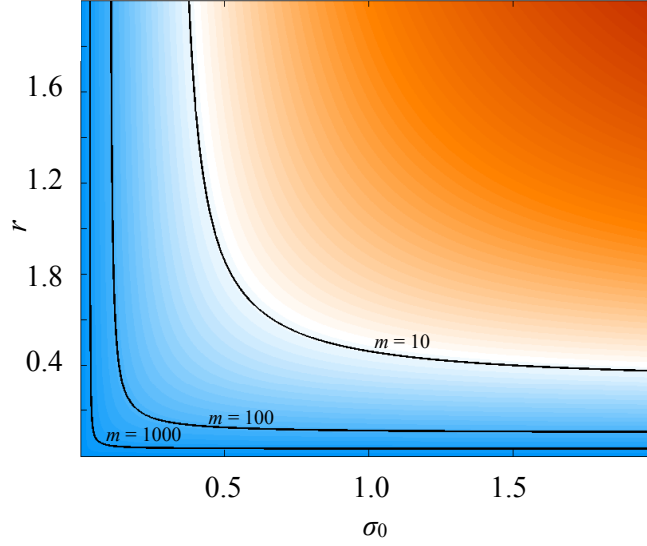


Figure 4: Covariance map for strong 4D-Var and optimal particle smoothing.

given state dimension, the values of r and σ_0 below the corresponding curve lead to a small $\|\Sigma\|_F$. We observe that, for a fixed m , a larger error in the prior knowledge (σ_0) can be tolerated if the error in the data is very small and vice versa. Similar observations were made in [16,17] in connection with the condition number in 3D-Var.

Variational data assimilation (strong 4D-Var) represents the conditional pdf by its mode, i.e. by a single point in the state space. The smaller is the ball on which the samples collect (i.e. the smaller the Frobenius norm of Σ), the more applicable is strong 4D-Var. Particle smoothers on the other hand construct an empirical estimate of the pdf via sampling. Since the target pdf is Gaussian, we can construct an optimal particle smoother (minimum variance in the weights) by sampling this Gaussian, so that the weights are constant (zero variance). It is clear that, for realistic conditions (small $\|\Sigma\|_F$) the optimal particle smoother can be expected to perform well,

regardless of the state dimension m , because it can efficiently represent the pdf one is interested in.

The situation is different for other particle smoothers. Consider, for example, the SIR-like particle smoother that uses $p(x_0)$ as its importance function. This filter produces weights whose negative logarithm is given by

$$\phi = \frac{1}{2} \sum_{j=1}^n (Z^j - HA^j x^0)^T R^{-1} (Z^j - HA^j x^0).$$

For $n = 1$, the variance of these weights depends on the Frobenius norm of the matrix $HA\Sigma_0 A^T H^T R^{-1}$, which has the upper bound

$$\|HA\Sigma_0 A^T H^T R^{-1}\| \leq \|H\|_F^2 \|A\|_F^2 \|\Sigma_0\|_F \|R^{-1}\|.$$

If we require that this upper bound is less than \sqrt{m} then we obtain (using $\sqrt{m} \leq \|A\|_F \|A^{-1}\|_F$) the condition

$$\|H\|_F^2 \|A\|_F^2 \|\Sigma_0\|_F \leq \|R\|,$$

which implies that the errors before we collect the data must be smaller than the errors in the data, which is unrealistic. In particular, for the simple example considered above we find that $\sigma_0 \leq r/\sqrt{m}$. We conclude that, as in particle filtering, particle smoothing is possible under realistic conditions only if the importance function is chosen carefully.

Note that the results we obtained here are different than those we would obtain if we would simply put $Q = 0$ in the Kalman filter formulas of section 2. It is easy to show that for $Q = 0$ the steady state covariance matrix converges to the zero matrix. What this means is that, with enough data, one can wait for steady state, and then accurately estimate the state at large n . What we have done in this section is to consider the consequences of having access to only a finite data set, i.e. making predictions before steady state is reached.

Finally, note that, in contrast to the sequential problem, the minimum variance of the weights of the smoothing problem is zero, whereas particle filters always produce non-zero variance weights. This variance is induced by the factorization of the importance function π , and since this factorization is not required in particle smoothing, this source of variance can disappear (or be reduced) by clever choice of importance functions.

5.2 The weak constraint problem

In the weak constraint problem (see e.g. [4]), one is interested in estimating the full state trajectory given the data, i.e. in the pdf

$$p(x^{0:n}|z^{1:n}) \propto \exp\left(-\frac{1}{2}(x^0 - \mu_0)^T \Sigma_0^{-1}(x^0 - \mu_0)\right) \\ \times \exp\left(-\frac{1}{2}\sum_{j=1}^n (z^j - Hx^j)^T R^{-1}(z^j - Hx^j)\right).$$

An easy calculation reveals that this pdf is Gaussian and its covariance matrix is

$$\Sigma^{-1} = \begin{pmatrix} \Sigma_0^{-1} + A^T \Sigma_1^{-1} A & -A^T Q^{-1} & \cdots & 0 \\ -Q^{-1} A & Q^{-1} + A^T Q^{-1} A + H^T R^{-1} H & -A^T Q^{-1} & \\ 0 & \ddots & \ddots & \ddots \\ \vdots & & & -A^T Q^{-1} \\ 0 & \cdots & -Q^{-1} A & Q^{-1} + H^T R^{-1} H \end{pmatrix}.$$

For the same arguments as before, data assimilation can only be successful if the Frobenius norm of Σ is moderate. This implies (again) a delicate balance condition between the errors in the prior knowledge ($\|\Sigma_0\|_F$), the errors in the model (1) ($\|Q\|_F$) and the errors in the data (2) ($\|R\|_F$).

As in the strong constraint problem, variational data assimilation (weak 4D-Var) represents this pdf by its mode (a single point) and this approximation is the more applicable, the smaller the Frobenius norm of Σ is. An optimal particle smoother can be constructed for this problem by sampling directly (zero variance weights) the Gaussian conditional pdf. For the same reasons as in the previous section, we can expect an optimal particle smoother to perform well under realistic conditions, but also can expect difficulties if the choice of importance function is poor.

6 Limitations of the analysis

We wish to point out limitations of the analysis above. To find the conditions for successful data assimilation we study the conditional pdf and we rely on the Kalman formalism to compute it. Since the Kalman formalism is only applicable to linear Gaussian problems, our results are at best indicative of the general nonlinear/non-Gaussian case. However, we believe that the general idea of that the probability mass must concentrate on a low-dimensional

manifold holds in the nonlinear case as well. Since Khinchin’s theorem is independent of our linearity assumption, and since we expect that correlations amongst the errors also occur in nonlinear models, one can speculate that the probability mass *does* collect on a low-dimensional manifold (under realistic assumptions on the noise). However finding (or describing) this manifold in general becomes exceedingly difficult and is perhaps best done on a case-by-case basis in which special features, or structures, in the model at hand can be exploited.

We have further assumed that all model parameters, including the covariances of the errors in the model and data equations, are known. If these must be estimated simultaneously (combined parameter and state estimation), then the situation becomes far more difficult, even in the case of a linear model equation (1) and data stream (2). It seems reasonable that estimating parameters using data at several consecutive time points (as is done implicitly in some versions of variational data assimilation or particle smoothing) would help with the parameter estimation problem and perhaps even with model specification.

Concerning particle filters, we have examined in detail only two choices of importance function, the one in SIR, where the samples are chosen independently of the data, and, at the other extreme, one where the choice of samples depends strongly on the data. There is a large literature on importance functions, see [9, 10, 12, 27, 35–38]; it is quite possible that other choices can outperform the optimal/implicit particle filter even in the present linear synchronous case once computational costs are taken into account. In nonlinear problems the optimal particle filter is hard to implement and the implicit particle filter is suboptimal, so further analysis may be needed to see what is optimal in each particular case (see also [36, 38] for approximations of the optimal filter).

More broadly, the analysis of particle filters in the present paper is not robust as assumptions change. For example, if the model noise is multiplicative (i.e. the covariance matrices are state dependent), then our analysis does not hold, not even for the linear case. Moreover, the optimal particle filter becomes very difficult to implement, whereas the SIR filter remains easy to use. Similarly, if model parameters (the elements of A or the covariances Q and R) are not known, simultaneous state and parameter estimation using an optimal particle filter becomes difficult, but SIR, again, remains easy to use. While the filters may not collapse in these cases, they may give a poor prediction. The existence of such important departures is confirmed by the fact that the ensemble Kalman filter and square root filter differ substantially in their performance. However, our analysis indicates that, if (1)

and (2) hold, the ensemble Kalman filter, the Kalman filter and the optimal particle filter are equivalent in the non-collapse region of the optimal filter.

Similarly, variational data assimilation or particle smoothing can be successful (and is indeed equivalent to Kalman filtering) if (1) and (2) hold. We expect that variational data assimilation and particle smoothing can be successful in the nonlinear case, provided that the probability mass concentrates on a low-dimensional manifold. In particular, particle smoothing has the potential of extending the applicability of Monte Carlo sampling to data assimilation, since the variance of weights due to the sequential problem formulation in particle filters is reduced (the data at time 2 may label what one thought was likely at time 1 as unlikely). This statement is perhaps corroborated by the success of variational data assimilation in numerical weather prediction.

Finally, it should be pointed out that we assumed throughout the paper that the model and data equations are “good”, i.e. that the model and data equations are capable of describing the *physical* situation one is interested in. It seems difficult in theory and practice to study the case where the model and data equations are incompatible with the (real) data one has collected. For example, it is unclear to us what happens if the covariances of the errors in the model and data equations are systematically under- or overestimated, i.e. if the various data assimilation algorithms work with “wrong” covariances.

7 Conclusions

We have investigated the conditions under which data assimilation is feasible, regardless of the algorithm used to do the assimilation. We quantified these conditions by defining an effective dimension of a Gaussian data assimilation problem and have shown that the boundedness of the effective dimension induces a balance condition for the errors in the model and data. This condition must be satisfied or else one cannot reach reliable conclusions about the process one is modeling, even when the (linear) model is completely correct. The balance condition is often satisfied for realistic models, i.e. the effective dimension is moderate, even if the state dimension is large.

The analysis was carried out in the linear synchronous case, where it can be done in some generality; we believe that this analysis captures the main features of the general case, but we have also discussed the limitations of the analysis.

Building on the results in [2, 5, 30, 31], we studied the effects of the effective dimension on particle filters in two instances, one in which the importance function is based on the model alone, and one in which it is based on both the model and the data. We have three main conclusions:

1. The stability (i.e., non-collapse of weights) in particle filtering depends on the effective dimension of the problem. Particle filters can work well if the effective dimension is small even if the true dimension is large (which we expect to happen often in practice).
2. A suitable choice of importance function is essential, or else particle filtering fails even when data assimilation is (in principle) possible with a sequential algorithm.
3. There is a parameter range in which the model noise and the observation noise are roughly comparable, and in which even the optimal particle filter collapses, even under ideal circumstances.

We have then studied the role of the effective dimension in variational data assimilation and particle smoothing, for both the weak and strong constraint problem. It was found that these methods too require a moderate effective dimension or else no accurate predictions can be expected. Moreover, variational data assimilation or particle smoothing may be applicable in the parameter range where particle filtering fails, because the use of more than one consecutive data set helps reduce the variance which is responsible for the collapse of the filters.

These conclusions are predicated on the linearity of the model and data equations, and on the assumption that the generative and data models are close enough to reality.

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